Quantum Computing Use Cases

Molecular Simulation for Application to Automotive Material Design

TOYOTA



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

Industry	Process Manufacturing
Process	research and development
Method	Simulation
Category	Gate*

Background

- **Large-scale computer simulations are becoming increasingly important in all aspects of automotive research and development, and the need for HPC (High Performance Computing) is growing.**
- As the Moore's Law factory of classical computing power is expected to die down, the promise of quantum computing is growing these days.
  - ✓ For example, while research and development related to functional materials is an essential element for achieving carbon neutrality, **research subjects related to all kinds of materials such as battery reactions** are known to be compatible with quantum computers.

Issues and motivation to be solved

- **Calculations of electronic states represented by the DFT method (density functional method)** are diversified in the research and development of automotive materials, and **quantum chemical calculations are used as a compass for material screening,** such as the design of electrode materials for lithium-ion batteries.
- Quantum computers are expected to improve prediction accuracy because they can treat **electron correlations (many-body interactions between electrons) more strictly** than existing DFT methods.
- In this verification, **TOYOTA and QunaSys collaborated to compare the actual thermodynamic behavior of liquid hydrogen in hydrogen storage for fuel cells and hydrogen engines with the existing DFT method and quantum computer in terms of the interaction between hydrogen molecules**

Reference: J-STAGE "Applicability of Quantum Computing to Automotive Materials Design" (https://www.jstage.jst.go.jp/article/jsaeronbun/54/1/54_20234032/_pdf/-char/ja)
*Gate（gate-based）: A computing approach in which operations are applied sequentially to qubits to perform calculations. Similar in concept to logic circuits in classical computers, it can address a wide range of problems.

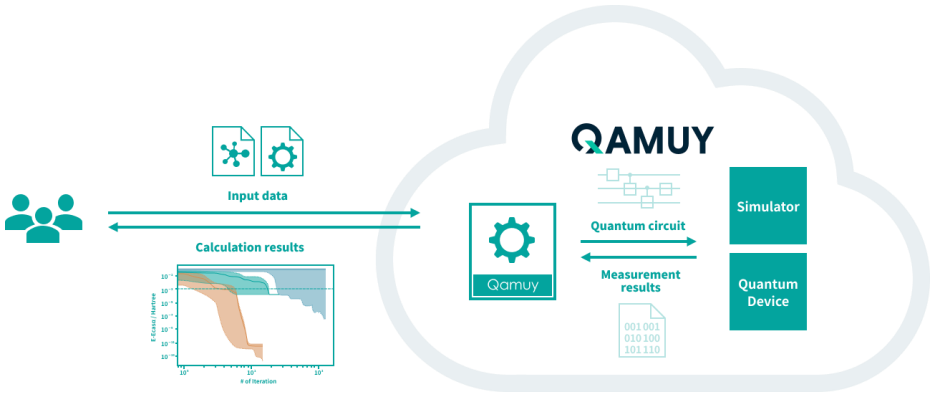
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Problem setting as a quantum computer

- **Van der Waals interaction between hydrogen molecules is taken up, and minute energy change between different hydrogen molecules is calculated** was performed as an object in which the effect of electron correlation may be conspicuous.
- As a calculation method of electronic state, **VQE utilizing quantum computer,** * **DFT method used in MI (material informatics) of method and classical computer** are mainly used.
- The electronic state calculation by the VQE method was performed using **QynaSys quantum chemical calculation cloud service Qamuy**.
  - ✓ **As a simulator of quantum computer (gate), Qulacs which can be implemented in Python base was used.**



How to Use Qamuy

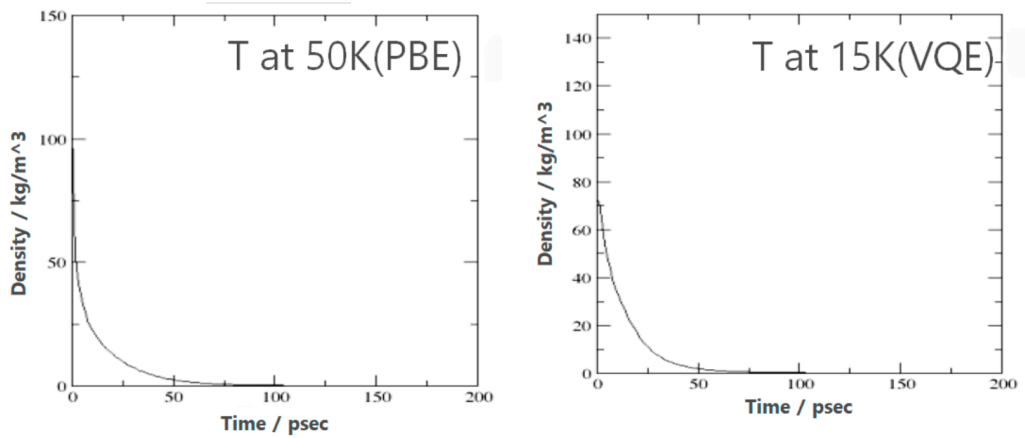
Reference: J-STAGE "Applicability of Quantum Computing to Automotive Material Design " (https://www.jstage.jst.go.jp/article/jsaeronbun/54/1/54_20234032/_pdf/-char/ja,), Qamuy" Flow image of using Qamuy " (https://qunasys.com/services/qamuy/) ", "How to use Qulacs, the world's fastest simulator " (https://dojo.qulacs.org/ja/latest/notebooks/3.1_Qulacs_tutorial.html)[LINK1]

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Expected business benefits

- Molecular dynamics simulations of the evaporation process of liquid hydrogen (3810 atoms) were performed by the classical DFT method (PBE, * and**) and the quantum VQE method,** while gradually increasing the temperature, and the temperature at which liquid hydrogen drastically reduces its density was measured.

- **The results obtained by the quantum VQE method are closer to the experimental ones.**
  - ✓ The measured boiling point of liquid hydrogen is about 20 K (Kelvin). Evaporation is observed at about 15 K by the quantum VQE method, while the classical DFT method at 50 K. The measured boiling point of liquid hydrogen is about 20 K.



Comparison of Hydrogen Vaporization Behaviors by Classical DFT (PBE) and Quantum VQE

Reference: J-STAGE "Applicability of Quantum Computing to Automotive Materials Design" (https://www.jstage.jst.go.jp/article/jsaeronbun/54/1/54_20234032/_pdf/-char/ja)

More use cases are available on our website. We invite you to explore them.
https://www.quantum-computing-use-cases.nedo.go.jp/english/

More Use Cases

New Energy and Industrial Technology Development Organization (NEDO)
AI and Robotics Department (e-mail: quantum_ai@ml.nedo.go.jp)

This collection of use cases was obtained as a result of the work commissioned by the New Energy and Industrial Technology Development Organization (NEDO) "Cyber-Physical Development Business of Quantum/Classical Hybrid Technology/Study of Use Case of Quantum Technology" and the “Post-5G Information and Communications System Infrastructure Reinforcement R & D Project (Quantum Industrialization)/Comprehensive Study for Promoting the Industrialization of Quantum Computers”.